```
=> d his

     (FILE 'HOME' ENTERED AT 12:30:36 ON 31 JAN 2002)

     FILE 'CAPLUS' ENTERED AT 12:31:03 ON 31 JAN 2002
L1             36 S DUMMY (W) ATOM
L2              6 S L1 AND HYDROGEN

=> d bib,abs 3,4
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=> s l1 and hydrogen
664946 HYDROGEN
4810 HYDROGENS
667747 HYDROGEN
(HYDROGEN OR HYDROGENS)
L2 6 L1 AND HYDROGEN

=> d bib,abs,kwic 1-6

L2 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2002 ACS
AN 1999:350219 CAPLUS
DN 131:141108
TI Improving efficiency of large time-scale molecular dynamics simulations of **hydrogen**-rich systems
AU Feenstra, K. Anton; Hess, Berk; Berendsen, Herman J. C.
CS Bioson Research Institute and Laboratory of Biophysical Chemistry, University of Groningen, Groningen, 9747 AG, Neth.
SO J. Comput. Chem. (1999), 20(8), 786-798
CODEN: JCCHDD; ISSN: 0192-8651
PB John Wiley & Sons, Inc.
DT Journal
LA English
AB A systematic anal. is performed on the effectiveness of removing degrees of freedom from **hydrogen** atoms and/or increasing **hydrogen** masses to increase the efficiency of mol. dynamics simulations of **hydrogen**-rich systems such as proteins in water. In proteins, high-frequency bond-angle vibrations involving **hydrogen** atoms limit the time step to 3 fs, which is already a factor of 1.5 beyond the commonly used time step of 2 fs. Removing these degrees of freedom from the system by constructing **hydrogen** atoms as **dummy atoms**, allows the time step to be increased to 7 fs, a factor of 3.5 compared with 2 fs. Addnl., a gain in simulation stability can be achieved by increasing the masses of **hydrogen** atoms with remaining degrees of freedom from 1 to 4 u. Increasing **hydrogen** mass without removing the high-frequency degrees of freedom allows the time step to be increased only to 4 fs, a factor of two, compared with 2 fs. The net gain in efficiency of sampling configurational space may be up to 15% lower than expected from the increase in time step due to the increase in viscosity and decrease in diffusion const. In principle, introducing **dummy atoms** and increasing **hydrogen** mass do not influence thermodynamical properties of the system and dynamical properties are shown to be influenced only to a moderate degree. Comparing the max. time step attainable with these methods (7 fs) to the time step of 2 fs that is routinely used in simulation, and taking into account the increase in viscosity and decrease in diffusion const., we can say that a net gain in simulation efficiency of a factor of 3 to 3.5 can be achieved.
RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT
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ST mol dynamics simulation **hydrogen** protein HPr

IT **Hydrogen** bond
(improving efficiency of large time-scale mol. dynamics simulations of **hydrogen**-rich systems such as proteins)

IT HPr (phosphocarrier protein)
Proteins, general, processes
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(improving efficiency of large time-scale mol. dynamics simulations of **hydrogen**-rich systems such as proteins)

IT Simulation and Modeling, physicochemical
(mol. dynamics; improving efficiency of large time-scale mol. dynamics simulations of **hydrogen**-rich systems such as proteins)

IT 1333-74-0, **Hydrogen**, processes 7732-18-5, Water, processes
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(improving efficiency of large time-scale mol. dynamics simulations of **hydrogen**-rich systems such as proteins)

L2 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2002 ACS

AN 1998:138725 CAPLUS

TI Quantum mechanical models of linear **hydrogen** bonds.

AU French, Alfred D.; Jursic, Branko S.

CS Southern Regional Research Center, U. S. Department Agriculture, New Orleans, LA, USA

SO Book of Abstracts, 215th ACS National Meeting, Dallas, March 29-April 2 (1998), CARB-039 Publisher: American Chemical Society, Washington, D. C.
CODEN: 65QTAA

DT Conference; Meeting Abstract

LA English

AB Chains of **hydrogen** bonds, as found in crystals of carbohydrates, have **hydrogen** bonds that are shorter and stronger than those in the water dimers in the vapor phase. Difficulties in modeling **hydrogen** bonds in carbohydrates with mol. mechanics (MM) methods are partially due to the lack of cooperativity in the MM force field. There is a need for data based on current quantum chem. methods so that MM methods can be accurately parameterized. Also, most previous work was based on cyclic water clusters that are not so relevant to condensed phases. In the current work, z-matrixes were built with 180.degree. O-H...O bond angles and **dummy atoms** were used with 0.degree. torsion angles to keep the arrays of water mols. from cyclizing. Calcns. used the 6-31 G(p,d) basis set using HF, MP2 and three d. functionals: B3LYP, BLYP and SVWN on one to seven water mols. As expected, the MP2 and B3LYP calcns. gave good geometries. In the B3LYP pentamer, the shortest H...O distance was 1.78 .ANG., while the dimer had a distance of 1.93 .ANG.. Bonds were also stronger in the chains, as shown by energy values.

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L2 ANSWER 3 OF 6 CAPLUS

AN 1995:790904 CAPLUS
DN 123:218959

TI A Molecular Dynamics Approach to Receptor Mapping: Application to the 5HT3 and .beta.2-Adrenergic Receptors

AU Gouldson, Paul R.; Winn, Peter J.; Reynolds, Christopher A.
CS Department of Chemistry and Biological Chemistry, University of Essex, Colchester/Essex, CO4 3SQ, UK

SO J. Med. Chem. (1995), 38(20), 4080-6
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English

AB A mol. dynamics-based approach to receptor mapping is proposed, based on the method of Rizzi (Rizzi, J. P.; et al. J. Med. Chem. 1990, 33, 2721). In Rizzi's method, the interaction energy between a series of drug mols. and probe atoms (which mimic functional groups on the receptor, such as **hydrogen** bond donors) was calcd. These interactions were calcd. on a three-dimensional grid within a mol. mechanics framework, and the min. in the grid were assocd. with the binding site on the receptor. In this extension, **dummy atoms**, bonded to the drug with appropriate mol. mechanics parameters, were placed at these min. The distances between the **dummy atom** sites were monitored during mol. dynamics simulations and plotted as distance distribution functions. Important distances within the receptor became apparent, as drugs with a common mode of binding share similar peaks in the distance distribution functions. In the case of specific 5HT3 ligands, the important donor-acceptor distance within the receptor has a range of .apprx.7.9-8.9 .ANG.. In the case of specific .beta.2-adrenergic ligands, the important donor-acceptor distances within the receptor lie between .apprx.7-9 .ANG. and between 8 and 10 .ANG.. These distance distribution functions were used to assess three different models of the .beta.2-adrenergic G-protein-coupled receptor. The comparison of the distance distribution functions for the simulation with the actual donor-acceptor distances in the receptor models suggested that two of the three receptor models were much more consistent with the receptor-mapping studies. These receptor-mapping studies gave support for the use of rhodopsin, rather than the bacteriorhodopsin template, for modeling G-protein-coupled receptors but also sounded a warning that agreement with binding data from site-directed mutagenesis expts. does not necessarily validate a receptor model.

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L2 ANSWER 4 OF 6 CAPLUS

AN 1994:95746 CAPLUS

DN 120:95746

TI Method of searching the structure of stable biopolymer-ligand molecule composite

IN Itai, Akiko; Yamada, Miho

PA Japan

SO PCT Int. Appl., 40 pp.
CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9320525	A1	19931014	WO 1993-JP365	19930326
	W: JP, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	EP 633534	A1	19950111	EP 1993-906826	19930326
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
PRAI	JP 1992-119484		19920327		
	WO 1993-JP365		19930326		

AB A method of searching the structure of a stable composite composed of a biopolymer and ligand mols. comprises: (1) covering all modes of **hydrogen** bonding between a biopolymer and ligand mols. by covering all of the possible combinations of matching between **dummy atoms** positioned at the **hydrogen**-bonding heteroatoms of the **hydrogen**-bonding functional groups of the biopolymer and the **hydrogen**-bonding heteroatoms of the ligand mols.; (2) estg. the modes of **hydrogen** bonding between the biopolymers and the ligand mols. and the conformations of the **hydrogen**-bonding portions of the ligand mols. at the same time by comparing the distance between the **dummy atoms** with that between the **hydrogen**-bonding heteroatoms; and (3) finding the structure of a biopolymer-ligand mol. composite by substituting the coordinates of all the atoms of the ligand mols. on the basis of the relation of matching between the **hydrogen**-bonding heteroatoms of the ligand mols. and the **dummy atoms** for each of the modes of **hydrogen** bonding and the conformations estd. in the second step into the coordinate

system of the biopolymer. This method permits the structure of a stable biopolymer-ligand mol. composite to be searched efficiently and accurately in a short time. The method is useful for designing pharmaceuticals, agrochems., or physiol. active compds. Thus, the method was used for detg. the stable structure of methotrexate (MTX)-dihydrofolic acid receptor (DHFR) complexes and DHFR-MTX-NADPH complexes.

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ST biopolymer ligand complex structure search; **hydrogen** bond biopolymer ligand structure analysis; drug design ligand biopolymer complex structure; agrochem design ligand biopolymer complex structure

IT Biopolymers
RL: BIOL (Biological study)
(complexes, with ligand, stable structure of, anal. of, **hydrogen** bonding energy calcn. method for)

IT Ligands
RL: BIOL (Biological study)
(conjugated, with biopolymers, stable structure of, anal. of, **hydrogen** bonding energy calcn. method for)

IT Receptors
RL: BIOL (Biological study)
(folic acid, stable structure of methotrexate binding to, searching of, **hydrogen** bonding energy calcn. method for)

IT 4033-27-6, Dihydrofolic acid
RL: ANST (Analytical study)
(receptor for, searching of stable structure of methotrexate binding to, **hydrogen** bonding energy calcn. method for)

IT 53-57-6D, NADPH, complexes with methotrexate and dihydrofolate receptor
RL: ANST (Analytical study)
(searching of stable structure of, **hydrogen** bonding energy calcn. method for)

IT 59-05-2D, Methotrexate, complexes with dihydrofolate receptor
RL: PRP (Properties)
(stable structure of, searching of, **hydrogen** bonding energy calcn. method for)

L2 ANSWER 5 OF 6 CAPLUS
AN 1992:147416 CAPLUS
DN 116:147416
TI Molecular modeling of protein-carbohydrate interactions. Docking of monosaccharides in the binding site of concanavalin A

AU Imberty, Anne; Hardman, Karl D.; Carver, Jeremy P.; Perez, Serge
CS Lab. Synth. Org., Fac. Sci. Tech., Nantes, 44072, Fr.
SO Glycobiology (1991), 1(6), 631-42
CODEN: GLYCE3
DT Journal
LA English

AB A general procedure is described for addressing the computer simulation of protein-carbohydrate interactions. First, a mol. mech. force field capable of performing conformational anal. of oligosaccharides has been derived by the addn. of new parameters to the Tripos force field; it is also compatible with the simulation of protein. Second, a docking procedure which allows for a systematic exploration of the orientations and positions of a ligand into a protein cavity has been designed. This so-called 'crankshaft' method uses rotations and variations of virtual bonds connecting, via **dummy atoms**, the ligand to the protein binding site. Third, calcn. of the relative stability of protein ligand complexes is performed. This strategy has been applied to search for all favorable interactions occurring between a lectin [Con A (I)] and Me .alpha.-D-mannopyranoside or Me .alpha.-D-glucopyranoside. For each monosaccharide, different stable orientations and positions within the binding site can be distinguished. Among them, one corresponds to very favorable interactions, not only in terms of **hydrogen** bonding, but also in terms of van der Waals interactions. It corresponds precisely to the binding mode of Me .alpha.-D-mannopyranoside into I as revealed by the 2.9 .ANG. resoln. of the cryst. complex (Derewenda Z.; et al., 1989). Some implications of the present modeling study with respect to the mol. basis of the specificity of the interaction of lectins with various monosaccharides are presented.

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L2 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2002 ACS
AN 1980:435395 CAPLUS
DN 93:35395
TI Orientation and intramolecular **hydrogen** bonding of nitro groups in the crystal structure of picric acid, C6H3N3O7
AU Srikrishnan, T.; Soriano-Garcia, M.; Parthasarathy, R.
CS Cent. Crystallogr. Res., Roswell Park Mem. Inst., Buffalo, NY, 14263, USA
SO Z. Kristallogr. (1980), 151(3-4), 317-23
CODEN: ZEKRDZ; ISSN: 0044-2968
DT Journal
LA English

AB Picric acid is orthorhombic, space group Pca21, with a 9.262(1), b 19.137(1), and c 9.714(1) .ANG.; d.(obsd.) = 1.78 and d.(calcd) = 1.768 for Z = 4 (2 mols/Z). The structure was solved by a combination of the multisoln. technique and the "**dummy atom**" method and refined by block-diagonal least-squares to a final R of 0.058. The 2 mols. in the asym. unit have different orientations of the nitro groups. In mol. I, the nitro groups are inclined by 17.0, 0.4, 7.7.degree. whereas the corresponding values in mol. II are 2.7, 5.2 and 20.3.degree. resp. In both the mols., there is an internal H bond from the OH group to the proximal O of an adjacent nitro group (O-H...O 2.572, 2.619 .ANG.). There appears to be no correlation between the C-N bond distance and the twist of the nitro groups from the mean Ph plane.

TI Orientation and intramolecular **hydrogen** bonding of nitro groups in the crystal structure of picric acid, $C_6H_3N_3O_7$

AB Picric acid is orthorhombic, space group Pca21, with a 9.262(1), b 19.137(1), and c 9.714(1) .ANG.; d.(obsd.) = 1.78 and d.(calcd) = 1.768 for Z = 4 (2 mols/Z). The structure was solved by a combination of the multisoln. technique and the "**dummy atom**" method and refined by block-diagonal least-squares to a final R of 0.058. The 2 mols. in the asym. unit have different orientations of the nitro groups. In mol. I, the nitro groups are inclined by 17.0, 0.4, 7.7.degree. whereas the corresponding values in mol. II are 2.7, 5.2 and 20.3.degree. resp. In both the mols., there is an internal H bond from the OH group to the proximal O of an adjacent nitro group (O-H...O 2.572, 2.619 .ANG.). There appears to be no correlation between the C-N bond distance and the twist of the nitro groups from the mean Ph plane.